

MTA Számítástechnikai és Automatizálási Kutató Intézet Budapest





MAGYAR TUDOMÁNYOS AKADÉMIA  
SZÁMITÁSTECHNIKAI ÉS AUTOMATIZÁLÁSI KUTATÓ INTÉZETE

PROGRAM PACKAGE SPARSE MATRICES

Irta:

Gergely József

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DR VAMOS TIBOR

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### Abstract

In the paper programs are investigated for the solution of six problems of linear algebra where the matrices of the problems are sparse ones. Linear systems of equations are solved in the first four programs, the eigenvalues are computed in the 5th and 6th program in the symmetric, non-symmetric or band cases. The inverse and determinant also are computed in the first program.

### 1. Introduction

A lot of methods and programs for the solution of the problems of linear algebra are known. In the books dealing with linear algebra or numerical methods there are sections in which the methods for the solution of systems of linear equations and matrix inversion are investigated. Moreover, the libraries of computer centers contain various programs to solve problems of linear algebra.

Large size main memories are needed in computers for the solution of large size problems. The solutions of large size problems are computed by means of back store, if the main memory is not enough for the solution. In this case the programs of solutions are more sophisticated and the computation takes more time because of the transfer between the memories, (see [1]).

Computer manipulation of large size matrices is often possible, because the matrix has a number of zero elements such that it is sparse. The subject of the paper is to make known some methods and some programs for the solution of linear equations with sparse matrices, for the inversion of sparse matrices, for the computation of determinant and eigenvalues of sparse matrices.

The main memory can prove to be small in case of a not very large computer even if we utilise possibilities of sparsity of large size matrices. Our programs /except the first one/ are made for small computers. The second, third and fourth programs during the computation use the back store /disc/ also to store the matrices, they have, however such an organization that the transfer times between the memories are minimal.

Some reviews about programs to handle sparse problems can be found in the libraries (see [3], [4], [8],). Generally these programs can be used only in large computers or there is possible to solve only small problems for being used in smaller computers.

Our programs are made in FORTRAN in the computer CDC 3300. We give the memory need at each program.



## 2. Problems and methods

The problems and the methods for their solution are investigated in this chapter. There are given the sparse matrix  $A = \{a_{ij}\}$ ,  $i, j = 1, \dots, n$  and the vector  $b = \{b_i\}$ ,  $i = 1, \dots, n$ . The problems are to solve the system of linear equation  $Ax = b$ , to invert the matrix  $A$  and to compute the eigenvalues of the matrix  $A$  and  $\det(A)$ .

Problem 1. is to solve the system of linear equation  $Ax = b$  or to compute the inverse  $A^{-1}$  and  $\det(A)$ .

The Crout method is used for solution. This is the following: the matrix  $A$  is factorized  $A = LR$  by means of Gauss elimination, where  $L$  is a lower triangular matrix,  $R$  is an upper triangular matrix. The equation after the factorization is

$$(2.1) \quad Ax = LRx = Ly = b.$$

The solution of the equation (2.1) is in two steps: the successive solutions of the following two equations

$$(2.2) \quad Ly = b, \quad Rx = y.$$

To solve the equations (2.2) is very simple and quick because it can be done by means of substitutions ( $L$  and  $R$  are triangular).

The equation  $AX = I$  is solved for inversion by means of the Crout method, where  $I$  is the unit matrix. After factorization  $A = LR$  the equation

$$AX = LRX = LY = I$$

is solved in two steps, we have to solve the equations

$$(2.3) \quad LY = \bar{I}, \quad RX = Y.$$

The equations (2.3) are solved by the successive substitution by columns and their solutions give us the columns of the inverse.

During the Gauss elimination the singularity is examined and the change of rows is done, if it is necessary. Menatime the determinant of the matrix is computed.

Problem 2 is to solve the system of linear equation  $Ax = b$  by means of a disc by the help of Gauss elimination.

The main diagonal of the matrix plays an important role during the Gauss elimination. The places "fill in" (see [9]) in the matrix follow the main diagonal and they can be marked out before the beginning of the elimination (see [1], [2], ).

This possibility is used in the program, too. By this means the program uses also some zero elements in the computation, but it becomes simpler.

Let us consider the left part of the matrix. Let  $j$  be the column index of the first nonzero element in the  $i$ -th row in the left side of the diagonal. The fill in in the  $i$ -th row /left of the diagonal/ can occur between the  $j$ -th and the diagonal columns. Similarly let us consider



the upper part of the matrix. Let the  $i$ -th row index of the first nonzero element in the  $j$ -th column be in the upper side of the diagonal. The fill in in  $j$ -th column /upper side of the diagonal/ can occur between the  $i$ -th and the diagonal rows. In this manner before having begun the elimination we could mark out in the matrix the places where the nonzero elements are in the beginning of the elimination or the nonzero elements can occur during the elimination. This reasoning is applied in Program 2 and this "marked part" of the matrix is used during the computation. We suppose that the marked part of the matrix does not hold in the main memory of computer. We cut the matrix into pieces by rows such that both pieces should be contained in the main memory of the computer. The pieces of the matrix are stored in disc, they are transferred from disc to main memory and the elimination is performed between pieces in the following way: Elimination is performed in the first piece, then elimination is performed in the second piece by means of the eliminated first piece, then elimination is performed in the third piece by means of eliminated first and second pieces etc. Each eliminated piece is rewritten to disc. Finally substitution is done by means of rewritten pieces and the solution is obtained. The [1] is employed by this method for the inversion of a matrix.

Problem 2 is to solve the system of linear equation

$$Ax = b \quad \text{in a band case.}$$

Let us in the matrix

$$a_{ij} = 0, \quad \text{if} \quad |i-j| > k$$

The solution of the equation is computed by means of a disc with Gauss elimination.

The first part of the band matrix

$$A_1 = \{a_{ij}\}, \quad i, j = 1, \dots, k$$

/that is the  $(k+1) \times (k+1)$  part of the band matrix/ is stored in the main memory, the other parts are stored in disc in the following way: there are the elements

$$a_{ij}, (i=k+1, j=2, 3, \dots, k+1), (j=k+1, i=k, k-1, \dots, 2)$$

in the first record, there are the elements

$$a_{ij}, (i=k+2, j=3, 4, \dots, k+2), (j=k+2, i=k+1, k, \dots, 3)$$

in the second record, etc.

The first elimination step is the elimination of the first column of the matrix  $A_1$  by means of the first row of the matrix  $A_1$ . Then the first row of the matrix is transferred to disc, the first column of the matrix was eliminated and the first record from disc is connected to matrix  $A_1$ . The new matrix /with size  $(k+1) \times (k+1)$  / is the  $A_1$  matrix and the previous steps are repeated in it. The difference is that after each step a new record from disc is connected to the eliminated part of the matrix. These steps are followed till each record from disc is connected to the part matrix. Then the substitution is

performed /that is the solution is obtained/ by means of the eliminated parts in disc.

Problem 4 is to solve the system of linear equations  $Ax = b$  in symmetric band case. Consider in matrix

$$a_{ij} = a_{ji} \quad \text{and} \quad a_{ij} = 0, \quad \text{if} \quad |i-j| > k.$$

The solution of the equation is computed by means of disc with the Cholesky method. The matrix  $A$  is factorized  $A = LR$  /where  $L$  and  $R$  are triangular matrices/ by means of the Cholesky method. Then the equations

$$(2.4) \quad Ly = b, \quad Rx = y$$

are solved by means of substitution. The program reserves an  $A_1$  place of size  $k(k+1)/2$  in the main memory for a part of the band matrix. All the band matrices are stored in a disc. The factorization is performed in  $A_1$  in  $n$  steps. Before each elimination step a row of band matrix from disc is connected to  $A_1$  and after each elimination step a factorized row from  $A_1$  is rewritten on disc. The factorised matrices are built up by means of this rewritten part. The substitution is performed by means of this rewritten part.

Problem 5 is the computation of the eigenvalues of a sparse symmetric matrix.

First the symmetrical variant of the Lanczos method is applied for a sparse symmetrix matrix  $A$ . This takes place as follows: (see [7], [10]): Starting from the normal vector  $V_1$  we compute

$$\begin{aligned}
 \alpha_k &= V_k^T A V_k \\
 W_{k+1} &= A V_k - \alpha_k V_k - \beta_{k-1} V_{k-1}, \quad (\beta_0 = 0) \\
 \beta_k &= \|W_{k+1}\|_2 \\
 V_{k+1} &= W_{k+1} / \beta_k
 \end{aligned}
 \tag{2.5}$$

for  $k=1, 2, \dots, n$ . The matrix

$$\tag{2.6} \quad T = \begin{vmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \beta_2 & \\ & \ddots & \ddots & \ddots \\ & & & \alpha_n \end{vmatrix}$$

is similar to matrix  $A$ . Then the eigenvalues of the matrix  $T$  are computed by means of the implicit QR method.

The application of the Lanczos - QR method for the computation of the eigenvalues of sparse matrices is very practical, because the computation of (2.5) is very easy in a sparse case too /whether in case of packed store form, or disc store/. The matrix  $T$  built up by (2.6) is tridiagonal and symmetric, therefore the application of QR method is possible in large size too. Nevertheless the method is stable.

The vectors  $V_k$  are orthonormalized vectors. However the orthogonalization is gone wrong during the computation. Therefore a re-orthogonalization is necessary /see [10]). A new orthogonal vector is generated, if  $V_k$  becomes 0.

Problem 6 is the computation of eigenvalues of a sparse nonsymmetric matrix.

First the Lanczos method is applied for the sparse matrix  $A$ . This is the following: Let  $C_0 = 0$  and vectors  $x_0 = y_0 = 0$ ,  $x_1$  and  $y_1$  are optional/but  $y_1^T x_1 \neq 0$ . We compute

$$\begin{aligned}
 b_k &= y_k^T A x_k / y_k^T x_k \\
 x_{k+1} &= A x_k - b_k x_k - c_{k-1} x_{k-1} \\
 y_{k+1} &= A^T y_k - b_k y_k - c_{k-1} y_{k-1} \\
 c_k &= y_{k+1}^T x_{k+1} / y_k^T x_k
 \end{aligned}
 \tag{2.7}$$

for  $k = 1, 2, \dots, n$ . The matrix

$$\tag{2.8} \quad T = \begin{vmatrix} b_1 & c_1 & & \\ 1 & b_2 & c_2 & \\ & \ddots & \ddots & \ddots \\ & & & b_n \end{vmatrix}$$

is similar to the matrix  $A$ . Then eigenvalues of the matrix  $T$  are computed by means of the bisection method /see [4], [5]). This is the following: The number of



the change of the sign in the sequence

$$(2.9) \quad 1, \det(B_1 - pI_1), \det(B_2 - pI_2), \dots, \det(B_n - pI_n)$$

is equal to the number of eigenvalues which is less than  $p$ . ( $B_i$  and  $I_i$  denote the left upper minor matrices of  $B$  and  $I$ .) The computation of sequence (2.9) is very fast for matrix (2.8).

The vectors  $x_k$  and  $y_k$  are biorthogonal vectors. However the biorthogonalism is gone wrong during the computation. Therefore a re-biorthogonalization is necessary /see [10] ). A new biorthogonal vector is generated if  $x_k$  or  $y_k$  becomes 0.

### 3. The programs

Six programs are discussed in this chapter for the solution of the six problems which were described in the previous chapter. The constructions of the input and output dates in the programs are different, therefore we discuss those separately.

The programs have been made in FORTRAN in computer CDC 3300. We give the store need in CDC CORE nomination:  
1 qp /quarter page/ = 512 words with 24 bites,  
1 seg /segment/ in disc = 20 qp.

Program 1: the solution of the system of sparse linear equation  $AX = B$ , or inversion of a sparse matrix  
/see Problem 1/.

The main program reads the parameters  $N, IP, IY, EPS$  in form /3I5, E16.7/ from cards, reads the nonzero elements  $a_{ij}$  of the matrix and their indexes from file 10 in form /3/2I5, F16.7//, then prints the input dates. The negative row index after the nonzero element denotes the end of dates. During the input the program built up the array  $AO(\cdot)$  from diagonal elements, the array  $A1(\cdot)$  from elements outside of the diagonal and the array  $M1(\cdot)$  from the row or column indexes of nonzero elements. The arrays  $A1$  and  $M1$  are in COMMON. The program uses the linked list manner for store (see [9]). After the input, the program

calls the corresponding SUBROUTINES and the solutions depending on the parameters are written out.

Parameter list:

N : order of the matrix A;

IP=0 : A=LR factorization;

IP= -1: A=LR factorization, computation and output of the inverse  $A^{-1}$  by columns;

IP=m : A=LR factorization, then m times: the right hand side is read from file 20, in form /5E15.5/, the solution is computed and written out;

IP < -1: the matrix is written out only;

NY=0 : the matrix is written out before and after the factorization;

NY=1 : the matrix is written out before the factorization;

NY=2 : the matrix is written out after the factorization;

NY=3 : the matrix is not written;

EPS : parameter for singularity investigation. If the pivot in the K-th step of elimination is less than EPS in absolute value the exchange of rows is performing. The program seeks the greatest element by column.

The SUBROUTINES:

LR factorizes the matrix A=LR;

CS performs the exchange of rows. A mark of exchange is given;

NYTAB executes the output of the matrix;

VISZ executes the back substitution to solve the equation

$$AX=B;$$

NYX prints the solution X.

The program using 84 qp in core, 5 seg in disc in CDC 3300 enables the computation of problems for  $N \leq 1000$ , the number of nonzeros  $\leq 5500$  /nonzeros at the start, or becoming nonzeros during computation/, the number of nonzeros in the rows  $\leq 200$ .

The list of the program:

THE PROGRAM SOLVES THE SYSTEM OF LINEAR EQUATIONS  $A \cdot X = R$  WITH SPARSE MATRIX.  
OR INVERTS A SPARSE MATRIX BY COLUMNS. THE PROGRAM COMPUTES THE  
DETERMINANT OF THE MATRIX IN BOTH CASES.  
METHOD - CROUT'S METHOD. THE PROGRAM USES ONLY THE NONZERO ELEMENTS  
OF THE MATRIX. THE DIAGONAL ELEMENTS ARE IN ARRAY A0, THE NON DIAGON-  
AL ELEMENTS ARE IN ARRAY A1, THEIR ROW OR COLUMN INDEXES ARE  
IN ARRAY M1.

# PARAMETERS :

N - NUMBER OF EQUATIONS :

IP = 0 - THE MATRIX IS FACTORIZED TO THE PRODUCT FORM  $A = L \cdot R$  :

IP = -1 - THE MATRIX IS FACTORIZED TO THE PRODUCT FORM, THE INVERSE  
OF THE MATRIX A IS COMPUTED AND WRITTEN OUT BY COLUMNS,

IP = M - THE MATRIX IS FACTORIZED TO THE PRODUCT FORM  $A = L \cdot R$ .

M TIMES : THE RIGHT-HAND-SIDE IS READ, THE EQUATION IS  
SOLVED, THE SOLUTIONS ARE WRITTEN OUT ;

IP . LT. -1- ONLY THE MATRIX IS WRITTEN OUT.

THE PARAMETER NY CONTROLS THE OUTPUT. THE MATRIX IS WRITTEN OUT IF :

NY = 0 BEFORE AND AFTER THE ELIMINATION ;

NY = 1 BEFORE THE ELIMINATION ;

NY = 2 AFTER THE ELIMINATION ;

NY = 3 NO WRITING OUT.

EPS CONTROLS THE SINGULARITY

```

DIMENSION I1(5),J1(5).
1A0(1000),M21(1000),M11(1000),B(1000),X(1000),MS(1000)
COMMON /20/ A1(5500),M1(11000)
REWIND 1
READ 1,N,IP,NY,EPS
1 FORMAT(3I5,F15.7)
PRINT 1,N,IP,NY,EPS
DO 9 I=1,N
  MS(I)=I
  M11(I)=I
  IN=I+N
9 M21(I)=IN
  M3=2*N
8 READ(1,10) ((I1(I),J1(I),R(I)),I=1,3)
  PRINT 2, ((I1(I),J1(I),R(I)),I=1,3)
2 FORMAT(1H,3(2I5,F16.7))
10 FORMAT(3(2I5,E16.7))
DO 4 K=1,3
  IF(I1(K)) 99,4,3
3 T=I1(K)
  J=J1(K)
  IF(I-J) 5,5,7
6 A1(I)=R(K)
  GOTO 4
5 M=M11(I)
  A1(M)=R(K)
  M11(I)=M3

```



```

M1(2*M)=J
M1(2*M-1)=M3
M3=M3+1
GOTO 4
7 M=M21(J)
A1(M)=B(K)
M21(J)=M3
M1(2*M)=I
M1(2*M-1)=M3
M3=M3+1
4 CONTINUE
GOTO 8
99 CONTINUE
IF (IP.GT.-2) GOTO 11
CALL NYTAB(N,M3,A0)
GOTO 98
11 CONTINUE
IF(NY.GT.1) GOTO 90
CALL NYTAB(N,M3,A0)
90 CONTINUE
CALL LR(N,M3,A0,M11,M21,EPS,MS,3,X)
IF(NY.EQ.1.OR.NY.EQ.3) GOTO 91
CALL NYTAB(N,M3,A0)
91 CONTINUE
IF(IP.EQ.0) GOTO 98
IF(IP.GT.0) GOTO 20
DO 39 M=1,N
DO 31 I=1,N
31 F(I)=0.
MM=MS(M)
B(MM)=1.
CALL VISZ(N,MM,IP,A0,3,X)
CALL NYX(N,M,X)
39 CONTINUE
20 REWIND 2
DO 29 M=1,IP

```

C  
C  
C

THE RIGHT HAND SIDE IS READING

```

READ(2,21) (B(I),I=1,N)
21 FORMAT(5E15.5)
CALL VISZ(N,M,IP,A0,3,X)
CALL NYX(N,M,X)
29 CONTINUE
98 CONTINUE
END

```

SUBROUTINE LR(N,M3,A0,M11,M21,EPS,MS,A5,A6)

THE SUBROUTINE LR FACTORIZED THE MATRIX TO THE PRODUCT FORM  $A=LR$

DIMENSION A0(N),M11(N),M21(N),MS(N),A5(N),A6(N),  
M5(200),M5(200)  
COMMON /20/ A1(5500),M1(11000)  
N1=N-1  
DET=1.  
DO 10 K=1,N1

IF THE PIVOT ELEMENT IN MODUL .LE. EPS THEN NEW PIVOT ELEMENT IS  
CHOSEN BY COLUMN AND EXCHANGE OF ROWS IS DONE.

IF (ABS(A0(K)).GT.EPS) GO TO 19  
CALL CS(K,N,M3,A0,M11,M21,MS,EPS)  
DET=-DET

19 K1=M1(2\*K-1)

K5=K

K2=1

1 IF (K1.EQ.0) GOTO 2

IF (M1(2\*K5).LE.K) GOTO 22

M5(K2)=M1(2\*K5)

A1(K5)=A1(K5)/A0(K)

A5(K2)=A1(K5)

K2=K2+1

22 K5=K1

K1=M1(2\*K1-1)

GOTO 1

2 KA=K+N

K1=M1(2\*KA-1)

K5=KA

K3=K2-1

K2=1

6 IF (K1.EQ.0) GOTO 5

M6(K2)=M1(2\*K5)

A6(K2)=A1(K5)

K5=K1

K1=M1(2\*K1-1)

K2=K2+1

GOTO 6

5 K4=K2-1

DO 7 I=1,K3

DO 7 J=1,K4

M1=M5(J)

M1=M5(J)

IF (M1.NE.MJ) GOTO 9

A0(M1)=A0(M1)-A5(I) A6(J)

GOTO 7

9 IF (M1.GT.MJ) GOTO 11

K5=M1

K1=M1(2\*M1)

```
K2=M1(2*MT-1)
13 IF(K2.EQ.0) GOTO 14
   IF(K1.EQ.MJ) GOTO 17
   K5=K2
   K1=M1(2*K2)
   K2=M1(2*K2-1)
   GOTO 13
12 A1(K5)=A1(K5)-A5(I) A6(J)
   GOTO 7
14 L=M11(MI)
   A1(L)=-A5(I)*A6(J)
   M1(2*L)=MJ
   M1(2*L-1)=MB
   M11(MI)=M3
   M3=M3+1
   GOTO 7
11 MA=M1+MI
   K1=M1(2*MA)
   K2=M1(2*MA-1)
   K5=MA
15 IF(K2.EQ.0) GOTO 16
   IF(K1.EQ.MI) GOTO 17
   K5=K2
   K1=M1(2*K2)
   K2=M1(2*K2-1)
   GOTO 15
17 A1(K5)=A1(K5)-A5(I) A6(J)
   GOTO 7
16 L=M21(MJ)
   A1(L)=-A5(I)*A6(J)
   M1(2*L)=MI
   M1(2*L-1)=MB
   M21(MJ)=M3
   M3=M3+1
7 CONTINUE
10 DET=DET*A0(K)
   DET=DET*A0(N)
   PRINT 18,DET
18 FORMAT(////7H DET=,F15.7)
   RETURN
END
```

SUBROUTINE CS(K,N,M3,A0,M11,M21,MS,EPS)

THE SUBROUTINE CS PERFORMS THE EXCHANGE OF ROWS.

DIMENSION A0(N),M11(N),M21(N),MS(N)

COMMON /20/ A1(5500),M1(11000)

KK=K

A=ABS(A0(K))

J=K+N

2 J1=M1(2\*J-1)

IF(J1.EQ.0) GOTO 3

IF(A.GE.ABS(A1(J))) GOTO 1

A=ABS(A1(J))

KK=J

1 J=J1

GOTO 2

3 IF(A.LT.EPS) GOTO 21

THE PIVOT ELEMENT IS CHOSEN FROM J2-TH ROW .

J2=M1(2\*KK)

AK=A0(K)

A0(K)=A1(KK)

A1(KK)=AK

M1(2\*KK)=J2

MS=MS(K)

MS(K)=MS(J2)

MS(J2)=MS

AJ=A0(J2)

A0(J2)=0

K1=K-1

DO 4 I=1,K1

I4=I+N

6 I1=M1(2\*I4-1)

I3=0

IF(I1.EQ.0) GOTO 4

IF(M1(2\*I4).EQ.K) I3=I4

IF(M1(2\*I4).EQ.J2) M1(2\*I4)=K

IF(I3.NE.0) M1(2\*I4)=I3

I4=I1

GOTO 6

4 CONTINUE

I=K

11 I1=M1(2\*I-1)

IF(I1.EQ.0) GOTO 10

I2=M1(2\*I)

IF(I2-J2) 7,8,13

8 A0(J2)=A1(I)

13 I=I1

GOTO 11

7 I4=I2+N

15 I5=M1(2\*I4-1)

```
IF (I5.EQ.0) GOTO 19
IF (M1(2*I4).NE.J2) GOTO 14
A=A1(I4)
A1(I4)=A1(I)
I5=M11(J2)
M11(I2)=M3
M1(2*I5-1)=M3
M3=M3+1
M1(2*I5)=I2
A1(I5)=A
GOTO 13
19 I5=M21(I2)
M21(I2)=M3
M1(2*I5-1)=M3
M3=M3+1
M1(2*I5)=J2
A1(I5)=A1(I)
GOTO 13
14 I4=M1(2*I4-1)
GOTO 15
10 I5=M11(J2)
M11(I2)=M3
M1(2*I5-1)=M3
M1(2*I5)=J2
M3=M3+1
A1(I5)=AJ
K1=K+1
K2=J2-1
DO 23 K3=K1,K2
  I=K3+V
  J1=K
25 IF (M1(2*J-1).EQ.0) GOTO 23
IF (M1(2*J).NE.J2) GOTO 24
27 IF (M1(2*J1).EQ.K3) GOTO 23
IF (M1(2*J1).GE.J2) GOTO 31
IF (M1(2*J1-1).EQ.0) GOTO 26
31 J1=M1(2*J1-1)
GOTO 27
24 J=M1(2*J-1)
GOTO 25
26 I5=M11(J2)
M11(I2)=M3
M1(2*I5-1)=M3
M3=M3+1
M1(2*I5)=K3
A1(I5)=A1(J)
A1(I)=0
23 CONTINUE
L1=M1(2*K-1)
L2=M1(2*K)
M1(2*K-1)=M1(2*J2-1)
M1(2*K)=M1(2*J2)
```



```

M1(2*I-1)=L1
M1(2*I)=L2
A=A1(I)
A1(K)=A1(J2)
A1(J2)=A
T=J2
28 I1=M1(2*I)
IF(I1.EQ.1) GOTO 29
IF(I1.GT.J2) GOTO 32
A1(I)=A
32 T=M1(2*I-1)
GOTO 28
29 CONTINUE
GOTO 16
21 CONTINUE
PRINT 20,N,K
20 FORMAT(12H SINGULARIS.2T5//)
STOP
16 CONTINUE
C THE MARK OF EXCHANGE .
C
PRINT 33,K,J2
33 FORMAT(7H CHERE:2I5)
I=M1(J2)
M1(I)=M1(K)
M1(K)=I
RETURN
END

```

```

SUBROUTINE NYTAB(N,M3,A0)
C THE SUBROUTINE NYTAB EXECUTES THE OUTPUT OF MATRIX
C
DIMENSION A0(N)
COMMON /20/ A1(500),M1(11000)
M5=2*M3
PRINT 1,N
PRINT 2,(A0(I),I=1,N)
PRINT 2,(A1(I),I=1,M3)
PRINT 3,(I,I=1,10)
PRINT 1,(M1(I),I=1,M5)
3 FORMAT(/10I9/)
1 FORMAT(10(I5,I4))
2 FORMAT(1H ,10F10.7)
RETURN
END

```

SUBROUTINE VISZ(N,M,IP,A0,B,Y)

THE SUBROUTINE VISZ EXECUTES THE BACK-SUBSTITUTION TO SOLVE THE EQUATION  $A \cdot X = B$ .

```

      DIMENSION A0(N),B(N),Y(N)
      COMMON /20/ A1(5500),M1(11000)
      DO 1 I=1,N
1    X(I)=0
      K=1
      IF (IP,IT,0) K=M
      DO 2 J=K,N
        Y(J)=B(J)/A0(J)
        IP=J+M
3    J1=M1(2*J3-1)
        J2=M1(2*J3)
        IF (J1.EQ.0) GOTO 2
        B(J2)=B(J2)-A1(J3)*X(J1)
        IP=J1
        GOTO 3
2    CONTINUE
      N1=N-1
      DO 5 I=1,N1
5    B(I)=X(I)
      DO 4 I=1,N1
        J1=N-I
        J=J1
6    J1=M1(2*I-1)
        J2=M1(2*I)
        IF (J1.EQ.0) GOTO 4
        B(J1)=B(J1)-A1(J2)*X(J2)
        J=J1
        GOTO 5
4    X(I1)=B(I1)
      RETURN
      END

```

SUBROUTINE NYX(N,M,X)

THE SUBROUTINE NYX PRINTS THE SOLUTION

```

      DIMENSION X(N)
      PRINT 1,M
      PRINT 2,(X(I),I=1,N)
1    FORMAT(//I5V)
2    FORMAT(5E13.9)
      RETURN
      END

```

Program 2 is for solution of a system of sparse linear equation by means of disc /see Problem 2/.

The program reads from file 10 the parameters  $N, N9, EPS$  in form /2I9, E15.5/, then the nonzero elements of the matrix and their indexes from file 20 in form /3/D16.9, 2I5/. The nonzero elements should be stored in file 20 by rows. After the last element there must be one negative row index. Finally the right-hand side is read from file 30 in form /5E15.9/.

The program during the reading by means of SUBROUTINE RENDEZ built up the sparse matrix in disc. During the computation the pieces of the matrix as unit are transferred between the main memory and disc memory. The program calls the SUBROUTINE SLED which computes the solution. Then the solution is written out.

Parameter list:

$N$  : the number of the equations;

$N9$  : the maximal size of one piece;

$EPS$  : parameter to investigate the singularity.

The program using 24 kb in core and 50 seg in disc is suitable for the solution of an equation with  $N \leq 1000$ ,  $N9 < 4000$ , number of pieces of nonzero elements  $\leq 100$ .

The list of the program:

```

C THE PROGRAM SOLVES THE SPARSE LINEAR SYSTEM WITH HELP OF THE
C SUBROUTINE SLED. THE PROGRAM CARRIES OUT THE INPUT FROM
C FILE 20.RY MEANS OF SUBROUTINE RENDEZ
C CONSTRUCTS THE MATRIX IN DISC, CALLS THE SUBROUTINE SLED AND
C PRINTS THE SOLUTION.
C PARAMETERS :
C N - THE NUMBER OF EQUATIONS ;
C N9 - MAX LENGTH OF A PART OF THE MATRIX ;
C EPS - THE PARAMETER FOR INVESTIGATION OF THE SINGULARITY
C THE PROGRAM USES THE FOLLOWING ARRAYS:
C M1(I) - THE NUMBER OF NONZERO ELEMENTS LEFT TO THE DIAGONAL IN THE
C I-TH ROW ;
C M2(I) - THE NUMBER OF NONZERO ELEMENTS RIGHT TO THE DIAGONAL IN
C THE I-TH ROW ;
C ID(K)+1 IS THE FIRST ROW INDEX IN THE K-TH PART OF THE MATRIX;
C ID(K+1) IS THE LAST ROW NUMBER IN THE K-TH PART OF THE MATRIX;
C M(J) : THE COLUMN INDEX OF THE NONZERO ELEMENTS RIGHT TO THE
C DIAGONAL, SUCCESSIVELY BY ROWS .
C
C THE PROGRAM USES SUCH A PART OF MATRIX IN WHICH THE ELEMENTS ARE NON-
C ZERO. OR NONZERO ELEMENTS CAN APPEAR DURING THE ELIMINATION .
C
C DIMENSION M1(1000),M2(1000),M3(1000),M4(1000),M(3000),ID(101),I3(
13),J1(3),IM(101),IA(101)
2,A(4000),B(1000),X(1000)
COMMON /10/ A,B,X,M
REWIND 10
READ(10,11) N,N9,EPS
PRINT 11,N,N9,EPS
REWIND 20
CALL RENDEZ (N,N9,M1,M2,M3,M4,ID,I3,J1,IM,IA)
REWIND 30
IM1=1
M3(1)=1
M4(1)=1
DO 41 I=2,N
M3(I)=M3(I-1)+M2(I-1)+M1(I)+1
41 CONTINUE
M41=2
DO 112 I=2,N
IF (I.LE.ID(M41)) GOTO 114
M4(I)=1
M41=M41+1
GOTO 112
114 M4(I)=M4(I-1)+M2(I-1)
112 CONTINUE
DO 34 K=1,N9
34 A(K)=0
C
C INPUT OF THE RIGHT SIDE . PERFORMED BY FORMAT 13.
C
C READ(30,13) (B(I),I=1,N)

```

```
ENDFILE 1
REWIND 1
ENDFILE 3
REWIND 3
ENDFILE 4
REWIND 4
CALL SLED(N, ID, M1, M2, M3, M4, N9, IM, IA, EPS)
```

```
C
C  OUTPUT OF THE SOLUTION
C
```

```
PRINT 27
PRINT 30, (I, X(I), I=1, N)
27 FORMAT(14H!THE SOLUTION: //)
11 FORMAT(2I8, E15.5)
13 FORMAT(5(E15.9))
30 FORMAT(15, E18.9)
END
```



```
SUBROUTINE RENDEZ (N,NQ,M1,M2,M3,M4,ID,I3,J1,IM,IA)
DIMENSION M1(1),M2(1),M3(1),M4(1),ID(1),I3(1),J1(1),IM(1),IA(1)
COMMON /10/ A(4000),R(1000),X(1000),M(3000)
```

C  
C THE SUBROUTINE RENDEZ BUILTS UP THE MATRIX IN DISC AND THE ARRAYS  
C M1,M2,ID,IA AND IM BY MEANS OF INPUT.  
C

```
L=1
ID1=1
ID(ID1)=L-1
K=0
KA=0
I8=0
K3=1
```

C  
C INPUT OF NONZERO ELEMENTS : A(I,J), I, J, WHERE I IS THE ROW \* J IS  
C THE COLUMN INDEX . PERFORMANCE BY FORMAT 9. THE END MARK IS I<0.  
C

```
6 READ (20,9) (X(I),I3(I),J1(I),I=1,3)
PRINT 9,(X(I),I3(I),J1(I),I=1,3)
DO 1 I=1,3
IF (I3(I)) 25,1,2
2 IF (I3(I)=1) 19,3,10
3 J2=J1(I)
J3=I3(I)-J2
IF (J3) 5,4,4
4 R(J2)=X(I)
IF (M1(L).LT.J3) M1(L)=J3
GOTO 1
5 K1=L+K3
I8=I8+1
K3=K3+1
R(K1)=X(I)
M3(K1)=J2
1 CONTINUE
GOTO 6
10 M2(L)=I8
K5=K+1
L1=L+1
L2=M1(L)+1
DO 7 J=1,L2
KA1=KA+J
KB=L-M1(L)+J-1
7 A(KA1)=0(KB)
KA=KA+L2
I8=0
GOTO 26
19 PRINT 18,L,I3(I),J1(I)
GOTO 1
25 I9=-1
GOTO 10
26 I4=L+1
```

```

J4=L
IF (M4(L).EQ.0) J4=L+1
14 IF (M3(I4).EQ.0.AND.M4(J4).EQ.0) GOTO 8
K=K+1
IF (M3(I4) = M4(J4)) 11,12,13
12 M(K)=M3(I4)
KA = KA+1
A(KA)=R(I4)
I4=I4+1
J4=J4+1
GOTO 14
13 IF (M4(J4).NE.0) GOTO 15
16 KA=KA+1
A(KA)=R(I4)
M(K)=M3(I4)
I4=I4+1
GOTO 14
15 M(K)=M4(J4)
KA=KA+1
J4=J4+1
GOTO 14
11 IF (M3(I4).EQ.0) GOTO 15
GO TO 16
8 DO 17 J=L,N
M3(J)=0
17 M4(J)=0
L=L+1
DO 20 J=K5,K
L2=L1+J-K5
20 M4(L2)=M(J)
K3=1
DO 33 J=1,N
33 B(J)=0
IF (KA.LT.N9.AND.I9.EQ.0) GOTO 3
IA(ID1)=KA
IM(ID1)=K
WRITE (1)(A(J),J=1,KA)
WRITE (2)(M(J),J=1,K)
WRITE (4)(M(J),J=1,K)
DO 24 J=1,KA
24 A(J)=0
ID1=ID1+1
ID(ID1)=L-1
DO 28 J=1,K
28 M(J)=0
K=0
KA=0
K3=1
IF (L.LT.N.AND.I9.EQ.0) GOTO 3
9 FORMAT (3(F16.9,2T5))
18 FORMAT (12H ORDER ERROR,3I5)
RETURN
END

```

SUBROUTINE SLED(N, ID, M1, M2, M3, M4, N9, IM, IA, EPS)

C THE SUBROUTINE SLED SOLVES THE SPARSE LINEAR SYSTEM. IT PERFORMS  
C THE GAUSS ELIMINATION AMONG PARTS OF THE SPARSE MATRIX. THE WHOLE  
C MATRIX IS IN DISC. PARTS ARE TRANSFERRED BETWEEN DISC AND MAIN  
C MEMORY.

```

      DIMENSION M1(1), M2(1), M3(1), M4(1), ID(1)
      1, A(4000), B(1000), X(1000), D(4000)
      2, MA(3000), MD(3000), IM(1), IA(1)
      COMMON /10/ A, B, X, MA
      J1=1
      IM1=1
      IM2=1
      J2=0
      1 IAL=IA(IM1)
      READ(1) (A(I), I=1, IAL)
      IM3=IM(IM1)
      IM1=IM1+1
      READ(3) (MA(I), I=1, IM3)
      I3=ID(J1)+1
      I4=ID(J1+1)
      IF(J1.EQ.1) GO TO 78
      J2=M3(I3-1)+M2(I3-1)
78 J5=J1-1
      IF (J5) 3,3,4
      4 DO 29 J4=1, J5
      I5=ID(J4)+1
      I6=ID(J4+1)
      IAL=IA(IM2)
      READ(2) (D(I), I=1, IAL)
      IM3=IM(IM2)
      IM2=IM2+1
      READ(4) (MD(I), I=1, IM3)
      DO 29 J6=I5, I6
      J7=0
      IF(J4.EQ.1) GO TO 79
      J7=M3(I5-1)+M2(I5-1)
79 DO 29 L2=I3, I4
      L3=J6+M1(L2)-L2
      L4=I5+L3
      IF(L3) 29,50,50
50 L5=M3(L2)+J6-L2-J7
      L7=M2(I6)
      DO 81 J=1, L7
      K=M4(J6)+J-1
      L6=MD(K)
      L14=M3(J6)+J-J7
      IF (L2-L6) 30,31,32
30 L8=M2(L2)
      DO 33 L=1, L8
      L9=M4(L2)+L-1

```

```

      IF (MA(L9)-L6) 33,34,34
33  CONTINUE
34  K1=M3(L2)+1
      GOTO 35
31  K1=M3(L2)
      GOTO 35
32  K1=M3(L2)+L6-12
35  K1=K1-12
      A(K1)=A(K1)-A(L5)*D(L14)
81  CONTINUE
      R(L2)=R(L2)-A(L5)*D(L16)
29  CONTINUE
3   DO 49 L2=I3,I4
      K1=M3(L2)-J-1
      IF (ABS(A(K1)).LT.FPS) GOTO 85
      R(L2)=R(L2)/A(K1)
      I13=L2+1
      DO 110 I=I13,I4
      IF (I-L2.GT.M1(I)) GOTO 110
      L6=M3(I)+L2-I-J2
      R(I)=R(I)-A(L6)*R(L2)
110  CONTINUE
      L4=M2(L2)
      DO 49 L=1,L4
      L5=M3(L2)+L-J2
      A(L5)=A(L5)/A(K1)
      DO 49 I=I13,I4
      IF (I-L2.GT.M1(I)) GOTO 49
      L6=M3(I)+L2-I-J2
      L7=M4(L2)+L-1
      L8=MA(L7)
      IF (I-L8) 38,39,40
39  L7=M3(I)
      GOTO 41
40  L7=M3(I)+L8-I
      GOTO 41
38  L9=M2(I)
      DO 42 J=1,L9
      L1=M4(I)+J-1
      IF (MD(L1)-L8) 42,43,43
42  CONTINUE
43  L7=M3(I)+J
41  L7=L7-12
      A(L7)=A(L7)-A(L6)*A(L5)
49  CONTINUE
      IF (ID(J1+1)-N) 46,47,47
46  IAL=IA(TM2)
      WRITE(2) (A(I),I=1,IAL)
      J1=J1+1
      ENDFILE 2
      REWIND 2
      REWIND 4

```

```
      IM2=1
      GOTO 1
47  ENDFILE 2
      IM3=IM(IM2)
      READ(4) (MD(I),I=1,IM3)
      GOTO 99
69  CALL BACKSTEP(1H2)
      CALL BACKSTEP(1H2)
      CALL BACKSTEP(1H4)
      CALL BACKSTEP(1H4)
      IA1=IA(IM2)
      IM3=IM(IM2)
      READ(2) (A(I),I=1,IA1)
      READ(4) (MD(I),I=1,IM3)
      IM2=IM2-1
99  L3=ID(J1)+1
      L4=ID(J1+1)
      L5=0
      IF(L3.LE.1) GO TO 76
      L5=M3(L3-1)+M2(L3-1)
76  L1=M3(N)-L5
      IF(L9) 63,64,64
64  L9=-1
      X(N)=B(N)
      L4=L4-1
63  DO 68 T=L3,L4
      K1=L4-T+L3
      X(K1)=R(K1)
      S=0
      L8=M2(K1)
      L7=M4(K1)
      DO 68 J=1,L8
      L6=L7+J-1
      L11=M3(K1)+J-L5
      I1=MD(L6)
68  X(K1)=X(K1)-A(L11)*Y(I1)
      J1=J1-1
      IF(J1) 67,67,69
85  PRINT 86,L2,I3,T4,K1,A(K1)
86  FORMAT(10H SINGULAR: ,4I5,E15,5)
67  RETURN
      END
```

Program 2 is for the solution of a system of linear equation with band matrix /see Problem 2/.

The solution is computed in SUBROUTINE SZALAG. We can call it:

CALL SZALAG (N,K,EPS) ,

where N is the number of equation. The bandwidth is  $2K+1$ . The parameter EPS investigates the singularity. If the pivot element in absolute value is less than EPS a mark is written out and the computation stops. There is a statement

COMMON /1/ A, B

in subroutine, where  $A(\cdot)$  is an array for the left upper part of the band matrix /the size is  $(K+1) \times (K+1)$ ,  $B(\cdot)$  is an array for the right hand side of equation. The other parts of the band matrix should be written in the file 1 in disc such as it was discussed in Problem 3. The solution is computed in array B and it is written out.

The subroutine using 80 op in core and 200 seg in disc is suitable for solving an equation with  $N \leq 7000$ ,  $K \leq 100$ , /but  $N.K < 3.5 \cdot 10^5$ /.

The list of the program:



SUBROUTINE SZALAG(N,K,EPS)

THE SUBROUTINE SZALAG SOLVES A SYSTEM OF EQUATION WITH BAND MATRIX .  
 THE FIRST  $(K+1)*(K+1)$  PART OF BAND IS IN ARDAY A AT THE BEGINING  
 THEN ONE ROW AND COLUMN ARE TRANSFERRED FROM FILE 1 SUCCESSIVELY  
 AND IT WILL BE CONNECTED WITH MATRIX A .  
 AFTER EACH ELIMINATION STEP ONE ROW IS WRITTEN TO THE FILE 2.  
 THE BACK-SUBSTITUTION IS CARRIED OUT WITH HELP OF FILE 2. THE RIGHT HAND  
 SIDE IS IN VECTOR B. ARRAYS A AND B ARE IN COMMON .  
 PARAMETER EPS: LOOKS FOR SINGULARITY . IN CASE OF SINGULARITY A CERTAIN  
 MARK IS WRITTEN OUT .  
 PARAMETERS : N IS THE NUMRER OF EQUATIONS ;  
 K IS THE HALF WIDTH OF BAND .  
 THE SOLUTION IS FORMED IN ARRAY B .

```

DIMENSION A(101*101)*B(7000)*C(201)
COMMON /1/ A//B
N1=N-1
K1=K+1
K2=K+K1
REWIND 1
DO 10 L=1,N1
  IF(ABS(A(1,1)).LT.EPS) GOTO 11
  A1=1/A(1,1)
  DO 1 J=2,K
1  A(1,J)=A1*A(1,J)
  B(L)=A1*B(L)
  DO 2 I=2,K1
    T1=L+I-1
    B(I1)=B(I1)-A(I,1)*B(I)
  DO 2 J=2,K
2  A(I,J)=A(I,J)-A(I,1)*A(1,J)
  WRITE(2) (A(1,J),J=2,K1)
  DO 3 I=1,K
    DO 3 J=1,K
3  A(I,J)=A(I+1,J+1)
  DO 4 I=1,K1
    A(K1,I)=0
4  A(I,K1)=0
  IF(L-N+K) 5,10,10
5  READ (1) (C(I),I=1,K2)
  DO 9 I=1,K
    A(K1,I)=C(I)
    J=K2-I+1
9  A(I,K1)=C(J)
    A(K1,K1)=C(K1)
10 CONTINUE
    L=N
    IF(ABS(A(1,1)).LT.EPS) GO TO 11
    B(N)=B(N)/A(1,1)
  ENDFILE 2
  CALL BACKSTEP(142)

```

```
DO 6 L=1,N1
  L1=N-L
  CALL BACKSTEP(142)
  READ(2) (A(1,I),I=1,K)
  CALL BACKSTEP(142)
  DO 6 I=1,K
    I1=L1+I
  6 B(L1)=B(L1)-A(1,I)*B(I1)
  GOTO 13
11 PRINT 12,L,A(1,1)
12 FORMAT(12H SZING.      :.15.F12.5)
13 CONTINUE
  RETURN
END
```

Program 4 is for the solution of a system of the linear equations with symmetric band matrix /see Problem 4/.

The program reads the parameters  $N, NI, EPS$  in form /2I5, F10/ from card, where  $N$  is the half width of band,  $NI$  is the number of equations,  $EPS$  investigates the singularity. If the pivot in Cholesky factorization is less then  $EPS$  in absolute value a mark is written out and the computation stops. The program reads in the way of rows the right parts of matrix from file 1, builds up in a one-dimensional array  $A$  /a  $(N+1) \times (N+1)$  size part of the band matrix/ and applies the Cholesky factorization for this part. After each step one row of the factorised matrix is rewritten into file 2 in disc. After  $NI$  steps the factor matrix is formed in file 2. Then the program reads the right hand side from file 3 and by means of (2.4) the solution is computed. The solution appears in array  $B$  and it is written out.

The program using 83 gp in core and 200 seg in disc is suitable for the solution of an equation with  $NK \leq 16110$ ,  $N \leq 179$ , /but  $N.NI < 10^6$ /.

The list of the program:

```

DIMENSION A(16110),R(16110),M(179),C(179)
EQUIVALENCE (A(1),R(1))
COMMON /10/ A
C
C THE PROGRAM SOLVES A SYSTEM OF LINEAR EQUATION WITH
C SYMMETRIC BAND MATRIX OF MEAN OF CHOLEVSKY METHOD
C
      READ 22,NK,N,FPS
22  FORMAT(2I5,F10.7)
      NN=N*(N+1)/2
      REWIND 1
      REWIND 2
      N2=N+1
      N3=NK+N
      M(1)=0
      M1=N
      DO 1 K=2,N
      M(K)=M(K-1)+M1
1  M1=M1-1
      DO 2 I=1,N
2  A(I)=0
      DO 10 KK=1,NK
      READ(1) (A(I),I=1,N)
      N1=N-1
      S=A(1)
      DO 3 I=2,N
      M1=M(I)+1
3  S=S-A(M1)*A(M1)
      S=SQRT(S)
      A(1)=S
      IF(S.LT.EPS) GOTO 9
      DO 4 I=2,N
      I1=N-I+1
      S1=A(I)
      DO 5 J=2,I1
      M1=M(J)+1
      M2=M(J)+I
5  S1=S1-A(M1)*A(M2)
4  A(I)=S1/S
      DO 6 I=1,N
      M1=M(I)+1
6  C(I)=A(M1)
      WRITE(2) (C(I),I=1,N)
      DO 7 K1=1,N1
      DO 7 L=1,K1
      K=N-K1
      I=M(K)+L+1
      J=M(K+1)+L
7  A(J)=A(I)
10 CONTINUE
      ENDFILE 2
      DO 8 I=1,N

```

```
8 R(I)=0
  READ(3) (B(I),I=N2,N3)
  REWIND 2
  DO 11 K=1,NK
    READ(2) (C(I),I=1,N)
    K1=N+K
    S=B(K1)
    DO 12 I=2,N
      K2=K1-I+1
12 S=S-R(K2)*C(I)
11 R(K1)=S/C(1)
    DO 13 K=1,NK
      CALL BACKSTEP(1H2)
      READ(2) (C(I),I=1,N)
      K1=N3-K+1
      CALL BACKSTEP(1H2)
      R(K1)=R(K1)/C(1)
      DO 14 I=1,N
        K2=K1-I
14 R(K2)=R(K2)-R(K1)*C(I+1)
13 CONTINUE
    PRINT 16,N,NK
16 FORMAT(12H A MEGOLDAS:./2I5//)
    PRINT 17,(R(I),I=N2,N3)
17 FORMAT(10F12.5)
    GOTO 19
    9 PRINT 19,KK,S
19 FORMAT(13H SZINGULARIS:./5E15.5)
18 CONTINUE
END
```

Program 5 is for the computation of eigenvalues of a symmetric sparse matrix /see Problem 5/.

The program reads the parameters N, EPS and EPS2 from card in form /I4,2E16.8/, where N is the order of matrix, EPS is the accuracy of eigenvalues and EPS2 investigates the singularity. Then reads N+1 number into array IS from file 2 in form /15I5/, which points to the beginning of the rows in arrays A and M. The nonzero elements of the right-hand side of the symmetric matrix and their column indexes are read from file 1 in form (4(I4,E16.8)) into array M and A. The nonzero elements in file 1 should be arranged by rows. The end of nonzero elements is denoted by a negative index.

The program executes the symmetric Lanczos method. The symmetric tridiagonal matrix is formed in array E(.) and D(.) . The SUBROUTINE AV (N,V,S) is used for the computation of product  $S=AV$ . After finishing the Lanczos method the explicite QR method is used for computation of eigenvalues of the tridiagonal matrix. It is done in SUBROUTINE QR (N, SMACHEPS,E,D,IER) . The eigenvalues of the matrix are formed in array B(.) . The serial number, the accuracy of eigenvalues and the eigenvalues are written out. The SUBROUTINE ORTSIM perform the re-orthogonalization and new orthogonal vector  $V_k$  is generated, if  $\|V_k\| \leq EPS2$ .

The program using 65 qp in core and 65 seg in disc is suitable for the computation of the eigenvalues of a matrix with  $N \leq 500$  and the number of nonzero elements  $\leq 5000$ .

The list of the program:



```

C
C THE PROGRAM COMPUTS THE EIGENVALUES OF A SYMMETRIC SPARSE MATRIX.
C THE SYMMETRIC LACZOS METHOD THEN THE IMPLICIT QR METHOD ARE USED.
C
  DIMENSION C(500),B(500),V(500),W(500),S(500),I1(5),A1(5)
  COMMON /10/ M(5000),A(5000),TS(500)
  REWIND 1
  REWIND 2

C
C THE INPUT OF PARAMETERS:
C N - IS THE ORDER OF MATRIX
C EPS - IS THE ACCURACY FOR EIGENVALUES
C EPS2 INVESTIGATES THE SINGULARITY
C
  READ 17,N,EPS,EPS2
  PRINT 17,N,EPS,EPS2
  N1=N+1

C
C THE ARRAY ELEMENT IS(I) LOOKS FOR THE FIRST NONZERO ELEMENT IN ROW I.
C
  READ(2,16) (IS(I),I=1,N1)
  K=1

C
C THE NONZERO ELEMENTS AND THEIR COLUMN INDEXES ARE READ FROM FILE 1
C
  CALL MILCO(IDO)
  PRINT 30,IDO
30 FORMAT(3I10)
  1 READ(1,15) (I1(I),A1(I),I=1,4)
  DO 2 I=1,4
    IF(I1(I)) 10,2,4
  4 M(K)=I1(I)
    A(K)=A1(I)
    K=K+1
  2 CONTINUE
  GO TO 1
10 DO 5 K=1,N
  5 V(K)=0.
  L3=1
  NK=1
  PRINT 16,(IS(I),I=1,N1)
  NN1=IS(N+1)-1
  PRINT 15,(M(I),A(I),I=1,NN1)
  V(1)=1
  V(N1)=1.
102 CONTINUE
  WRITE(3) (V(I),I=1,N1)
  C(1)=0
  DO 6 K=1,N
    NK1=K+1
    L4=1
    CALL AV(N,V,S)
    DO 7 L=1,N
  7 B(K)=B(K)+V(L)*S(L)
    DO 8 L=1,N
  8 W(L)=S(L)-B(K)*V(L)-C(K)*W(L)

```

```

CALL ORTSIM(N,K,W,S,C,EPS2,T,L3,L4)
IF(L4.LT.0) GOTO 106
DO 11 L=1,N
  D=V(L)
  V(L)=W(L)/T
11 W(L)=D
6 CONTINUE
106 IS=NK
  NK=NK+1
  C(K+1)=0
  PRINT 13,(I,C(I),B(I),I=IS,NK1)
  NK2=NK1-IS
  DO 121 I=1,NK2
    I6=IS+I-1
    C(I+1)=C(I6+1)
121 R(I)=R(I6)
  CALL QR(NK2,EPS,C,B,IFR)
C
C THE EIGENVALUES END THEIR ACCURACY ARE WRITTEN OUT
C
  DO 124 I=1,NK2
    I6=NK2-I+IS
    I7=NK2-I+1
    C(I6)=C(I7)
124 R(I6)=B(I7)
  NK3=NK2-1+IS
  PRINT 123,(I,C(I),B(I),I=IS,NK3)
  PRINT 130
  IF(K.GE.N) STOP
C
C A NEW ORTHOGONAL VECTOR IS GENERATED , IF W(.) IS SMALL
C
  L3=L3+1
  L2=L3
  DO 120 I=1,N
    C(I)=0.
120 R(I)=0.
  IF(L3.GT.N) GOTO 28
  DO 111 L=L2,N
    DO 12 I=1,N
      W(I)=0
      W(L)=1.
      REWIND 3
      DO 113 I=1,K
        READ(3) (S(J),J=1,N1)
        U=0
        DO 114 J=1,N
          U=U+S(J)*W(J)
114 CONTINUE
      Z=U/S(N1)
      DO 105 J=1,N
        W(J)=W(J)-Z*S(J)
105 W(J)=W(J)-Z*S(J)
113 CONTINUE

```

```
F=0
DO 116 I=1,N
116 F=F+W(I)*W(I)
T=SQRT(F)
DO 117 I=1,N
117 V(I)=W(I)/T
T=1.
V(N1)=T
WRITE(3) (V(I),I=1,N1)
IF(T.GT.EPS) GOTO 6
L3=L3+1
111 CONTINUE
28 PRINT 118,K,EPS,T
STOP
118 FORMAT(13H W EQUAL ZERO,I5,2E15.5)
123 FORMAT (4H-EIG,I4,2E20.10)
13 FORMAT(1H0,I5,2E18.9)
15 FORMAT(4(I4,E16.9))
16 FORMAT (15I5)
17 FORMAT(I4,2E16.9)
130 FORMAT(1H-)
END
SUBROUTINE QR(N,SMACHEPS,F,D,IER)
DIMENSION E(1),D(1)
C
C THE SUBROUTINE QR COMPUTES THE EIGENVALUES BY MEAN OF QR METHOD FOR THE
C THREE DIAGONAL MATRIX.
C
IER=0
DO 1000 I=2,N
1000 F(I-1)=E(I)
E(N)=0
K=N-1
DO 1001 L=1,N
J=0
1002 DO 1003 M=L,K
IF(ABS(E(M)).LE.SMACHEPS*(ABS(D(M))+ABS(D(M+1)))) GOTO 1004
1003 CONTINUE
M=N
1004 P=D(L)
IF(M.EQ.L) GOTO 1001
IF(J.EQ.30) GOTO 1005
```

```

J=J+1
G=(D(L+1)-P)/(2*E(L))
R=SQRT(1.+G*G)
Q=1.
IF(G.LT.0.) Q=-1.
G=D(M)-P+E(L)/(G+Q*R)
S=1.
C=1.
P=D(M)
MM=M-1
DO 1006 II=L,MM
I=M-1+L-II
F=S*F(I)
R=C*F(I)
IF(ABS(F).LT.ABS(G)) GOTO 1007
C=G/F
R=SQRT(1.+C*C)
E(I+1)=F*R
S=1./R
C=C/R
GOTO 1008
1007 C=F/G
R=SQRT(1.+C*C)
E(I+1)=G*R
S=C/R
C=1./R
1008 F=C*D(I)-S*B
G=C*R-S*P
R=D(I)+P
P=C*F-S*G
G=S*F+C*G
D(I+1)=R-P
1006 CONTINUE
D(L)=P
E(L)=G
F(M)=0
GOTO 1002
1001 CONTINUE
DO 1009 I=1,N
K=I
P=D(I)
III=J+1
DO 1010 J=III,N
IF(D(J).GE.P) GOTO 1011
K=J
1010 P=D(J)
1011 IF(K.EQ.I) GOTO 1012
D(K)=D(I)
D(I)=P
1012 CONTINUE
1009 CONTINUE
RETURN
1005 IER=1
RETURN
END

```

```
SUBROUTINE AV(N,V,S)
  DIMENSION V(1),S(1)
  COMMON /10/ M(5000),A(5000),IS(500)
```

C  
C THE SUBROUTINE AV COMPUTES THE PRODUCT  $S=A*V$ .  
C

```
  DO 1 K=1,N
    S(K)=0
    K1=IS(K)
    K2=IS(K+1)-1
    DO 2 I=K1,K2
      J=M(I)
2    S(K)=S(K)+A(I)*V(J)
    K3=K-1
    DO 3 I=1,K3
      K1=IS(I)
      K2=IS(I+1)-1
      DO 4 J=K1,K2
        IF (M(J).EQ.K) GOTO 5
4      CONTINUE
3    CONTINUE
    GOTO 1
5    S(K)=S(K)+A(J)*V(I)
    GOTO 3
1    CONTINUE
  RETURN
  END
  SUBROUTINE ORTSIM(N,K,W,S,C,EPS,T,L3,L4)
  DIMENSION W(1),S(1),C(1)
```

C  
C THE SUBROUTINE ORTSIM PERFORMS THE RE-ORTHOGONALIZATION OF THE MATRIX  
C

```
  REWIND 3
  DO 1 L=1,K
    Z1=0
    N1=N+1
    READ(3) (S(J),J=1,N1)
    DO 2 I=1,N
2    Z1=Z1+S(I)*W(I)
    Z2=Z1/S(N1)
    DO 3 I=1,N
3    W(I)=W(I)-Z2*S(I)
1    CONTINUE
    F=0
    DO 18 L=1,N
18    F=F+W(L)*W(L)
    T=SQRT(F)
    C(K+1)=T
    PRINT 19,N,K,T,F,S(N1),Z1,Z2
19    FORMAT(2I4,5E16.4)
    IF (T.GE.EPS) GOTO 7
    L4=-1
7    CONTINUE
    DO 20 I=1,N
20    W(I)=W(I)/T
    T=1
    W(N1)=T
    WRITE(3) (W(I),I=1,N1)
9    FORMAT(3I5,3E15.5)
  RETURN
  END
```

Program 6 is for the computation of eigenvalues of a nonsymmetric sparse matrix /see Problem 6/.

The program reads the parameters  $N, R1, R2, EPS, EPS1$  from the card in form  $(I5, 4F15.8)$ , where  $N$  is the order of matrix,  $EPS$  is the accuracy of eigenvalues,  $EPS1$  investigates the singularity. The nonzero elements of the matrix and their column index are read from file 2 in form  $(4(I4, E16.9))$ . The nonzero elements in file 1 should be arranged by rows, the program reads  $N+1$  number from file 1 which points to the place of the first nonzero in each row in matrix. The end of nonzero elements is marked by a negative index.

The program executes the Lanczos method. The SUBROUTINE AX  $(N, S, X)$  and SUBROUTINE AY  $(N, S, Y)$  are used for computations of products  $S=AV$  and  $S=A^T Y$ . The tridiagonal matrix is formed in array  $B(.)$  and  $C(.)$ , /the third array consists of ones/. The SUBROUTINE SEAT  $(N, R1, R2, I9, S, EPS)$  and SUBROUTINE SAJS2  $(N, P, NV)$  compute the eigenvalues of the tridiagonal matrix belonging to the interval  $(R1, R2)$  by means of the bisection method. The eigenvalues are formed in array  $B(.)$  in COMMON and they are written out.

The SUBROUTINE ORTOG performs the re-biorthogonalisation of the vectors.

If  $|C_k| < EPS1$  in (2.7) the matrix decompose to parts. The program computes the eigenvalues of the first part, new biorthogonal vectors are computed and the computation is continued.



The program using 71 qp in core and 115 seg in disc is suitable for the computation of the eigenvalues of a matrix with N 500 and the number of nonzero elements 5000.

The list of the program:

```

3
3 THE PROGRAM COMPUTES THE REAL EIGENVALUES BELONG IN INTERVAL (R1,R2)
3 THE LANCZOS METHOD THEN THE BISECTION METHOD ARE USED.
3
3 THE INPUT OF PARAMETERS:
3 N - IS THE ORDER OF MATRIX
3 EPS - IS THE ACCURACY FOR EIGENVALUES
3
3   DIMENSION IS(500),IO(5000),A(5000),B(500),C(500),X1(50
3   10),X2(500),Y1(500),Y2(500),S(500)
3   COMMON /1/ B,C /2/ IS,IO,A
3   READ 1,N,R1,R2,EPS,EPS1
3   PRINT 1,N,R1,R2,EPS,EPS1
3   N1=N+1
3   N2=N-1
3   REWIND 1
3   REWIND 2
3   L3=2
3   I1=1
3   READ(1,9) (IS(I),I=1,N1)
3   I2=IS(N+1)-1
3
3 THE NONZERO ELEMENTS AND THEIR COLUMN INDEXES ARE READ FROM FILE 2
3 THE ARRAY ELEMENT IS(I) LOOKS FOR THE FIRST NONZERO ELEMENT IN ROW I.
3
3   READ(2,10) (IO(I),A(I),I=1,I2)
3   PRINT 10,(IO(I),A(I),I=1,I2)
3   DO 50 L=1,N
3   DO 11 I=1,N
3   Y1(I)=0.
3   X1(I)=0.
3   X2(I)=0
3   Y2(I)=0
3 11 CONTINUE
3   X1(L)=1.
3   Y1(L)=1.
3   X1(N1)=1.
3   WRITE(3) (X1(I),I=1,N1)
3   WRITE(4) (Y1(I),I=1,N)
3   C(1)=0
3   S1=0
3   DO 12 I=1,N
3 12 S1=S1+X1(I)*Y1(I)
3   DO 19 K=1,N
3   CALL AX(N,S,X1)
3   S2=0
3   DO 13 I=1,N
3 13 S2=S2+Y1(I)*S(I)

```

```

PRINT 25,S1,S2
B(K)=S2/S1
DO 14 I=1,N
14 X2(I)=S(I)-B(K)*X1(I)-C(K)*X2(I)
CALL AY(N,S,Y1)
DO 15 I=1,N
15 Y2(I)=S(I)-B(K)*Y1(I)-C(K)*Y2(I)
CALL ORTOG(N,K,X2,Y2,EPS1,M,S3,SX,SY,L3)
I2=K+1
IF(M.LT.0) C(K+1)=0
IF(M.EQ.0) GOTO 60
GOTO 51
61 C(K+1)=S3*SY*SX/S1
161 S1=S3
DO 17 I=1,N
E=X1(I)
X1(I)=X2(I)
X2(I)=E
E=Y1(I)
Y1(I)=Y2(I)
17 Y2(I)=E
19 CONTINUE
IF(L.EQ.N) GOTO 21
GOTO 51
51 PRINT 10,L,S1,K
51 CONTINUE
I4=K-I1+1
PRINT 25,(B(I),C(I),I=I1,I2)
DO 18 I=1,N
18 C(I)=C(I+1)
DO 41 I=I1,I2
I3=I-I1+1
B(I3)=B(I)
C(I3)=C(I)
41 CONTINUE
R3=R1
R4=R2
CALL SEAT (I4,R3,R4,NS,S,EPS)
3
C THE EIGENVALUES ARE WRITTEN OUT
3
DO 142 I=I1,I2
I3=I2-I+1
I5=I2-I+I1
142 S(I5)=S(I3)
I7=I1+NS-1
PRINT 1,NS
PRINT 22,(I,S(I),I=I1,I7)
I1=I2
IF(K.GE.N) GOTO 24

```

```

      DO 42 I=1,N
      X1(I)=0.
42  Y1(I)=0.
      GOTO 160
20  PRINT 23,L,S1
24  CONTINUE
25  FORMAT(2E18.9)
      9  FORMAT (15I5)
11  FORMAT (4(I4,E16.9))
23  FORMAT(7H SZING:,I5,E15.5)
22  FORMAT(4H-EIG,I5,E18.9)
      1  FORMAT(I5,4E15.8)
      END
      SUBROUTINE AX(N,S,X)
      DIMENSION S(1),X(1)
      COMMON /2/ IS(500),IO(5000),A(5000)
C
C  THE SUBROUTINE AX COMPUTES THE PRODUCT S=A*X.
C
      DO 1 I=1,N
      S(I)=0
      KK=IS(I)
      KV=IS(I+1)-1
      DO 1 K=KK,KV
      J=IO(K)
1  S(I)=S(I)+A(K)*X(J)
      RETURN
      END
      SUBROUTINE AY(N,S,Y)
      DIMENSION S(1),Y(1)
      COMMON /2/ IS(500),IO(5000),A(5000)
C
C  THE SUBROUTINE AY COMPUTES THE PRODUCT S=Y*A
C
      DO 1 J=1,N
      S(J)=0
      DO 1 I=1,N
      IK=IS(I)
      IV=IS(I+1)-1
      DO 3 K=IK,IV
      IF (IO(K).EQ. J) GOTO 4
3  CONTINUE
1  CONTINUE
      GOTO 5
4  S(J)=S(J)+A(K)*Y(I)
      GOTO 1
5  RETURN
      END

```

```

SUBROUTINE SEAT(N,R1,R2,I9,S,EPS)
DIMENSION S(1)
C
C THE SUBROUTINE SEAT COMPUTES THE BISECTION METHOD
C
      NS=1
      CALL SAJS2(N,R1,N1)
      CALL SAJS2(N,R2,N2)
      PRINT 13,N,N1,N2,R1,R2
      IF(N2-N1) 1,1,2
C
C A MARG IS WRITTEN OUT IF EIGENVALUES ARE NOT IN INTERVAL (R1,R2)
C
      1 PRINT 3,R1,R2
        I9=0
        GOTO 1
      2 I9=N2-N1
C
C IT IS WRITTEN OUT HOW MANY EIGENVALUES ARE IN INTERVAL (R1,R2)
C
      PRINT 4,I9,R1,R2
      5 CONTINUE
      IF(R2-R1-EPS.LE.0.) GOTO 20
      P=(R1+R2)/2
      CALL SAJS2(N,P,N3)
      IF(N2-N3) 7,7,8
      7 R2=P
        GOTO 5
      8 IF(N3-N1) 21,21,22
      21 R1=P
        GOTO 5
      22 R3=P
      23 P=(R3+R2)/2
      IF(R2-R3-EPS.LE.0.) GOTO 20
      CALL SAJS2(N,P,N4)
      IF(N2-N4) 19,19,19
      19 R2=P
        GOTO 23
      18 R3=P
        GOTO 23
      2: S(NS)=P
        IF(NS.EQ.I9) GOTO 10
        NS=NS+1
        R2=P-2*EPS
        N2=N2-1
        GOTO 5
      10 CONTINUE
      13 FORMAT(3I5,2E16.6)
      3 FORMAT(23H IS NOT EIGENVALUE IN (,2E15.6,2H))
      4 FORMAT(115,21H EIGENVALUES ARE IN (,2E15.6,2H))
      RETURN
      END
```

```

SUBROUTINE SAJS2(N,P,NV)
COMMON /1/ B(500),C(500)
LOGICAL L

```

```

C SUBROUTINE SAJS2 COMPUTES THE NUMBER OF CHANGE OF SIGN IN THE SEQUENCE
C OF MINORS.
C

```

```

    NV=0
    L=.TRUE.
    D1=1.
    D2=B(1)-P
    IF (D2) 3,5,5
3   L=.NOT.L
    NV=1
5   CONTINUE
    DO 1 I=2,N
    D=D2*(B(I)-P)-C(I-1)*D1
    D1=D2
    D2=D
    IF (L.AND.D.GE.0..OR..NOT.L.AND.D.LT.0) GOTO 1
    NV=NV+1
    L=.NOT.L
1   CONTINUE
2   FORMAT(I5,2E16.7)
    RETURN
    END
    SUBROUTINE ORTOG(N,K,X2,Y2,EPS,M,S3,S1,S2,L3)
    DIMENSION X2(1),Y2(1),U(500),V(500)

```

```

C THE SUBROUTINE ORTOG PERFORMS THE RE-ORTHOGONALIZATION OF THE MATRIX
C

```

```

    REWIND 3
    REWIND 4
    M=J
    DO 1 L=1,K
    Z1=J
    Z2=0
    NL=N+1
    READ(3) (U(J),J=1,N1)
    READ(4) (V(J),J=1,N)
    DO 2 I=1,N
    Z1=Z1+V(I)*X2(I)
    Z2=Z2+U(I)*Y2(I)
2   CONTINUE
    Z5=Z1/U(N1)
    Z6=Z2/U(N1)
    DO 3 I=1,N
    X2(I)=X2(I)-Z5*U(I)
3   Y2(I)=Y2(I)-Z6*V(I)
1   CONTINUE
    L2=L3
    DO 17 L=L2,N
    S1=0
    S2=0
    DO 4 I=1,N
    S1=S1+X2(I)*X2(I)
4   S2=S2+Y2(I)*Y2(I)

```



3  
3  
C  
C

THE SUBROUTINE GENERATES A NEW BIORTOGONAL VECTORS  
IF X2 OR Y2 IN NORM LES THEN EPS.

```
PRINT 99,N,K,S1,S2,U(N1),Z5,Z6
99 FORMAT(2I5,5E12.4)
IF (S1.GE.EPS.AND.S2.GE.EPS) GOTO 15
IF (K.EQ.N) GOTO 97
M=-1
DO 6 I=1,N
6 X2(I)=0
X2(L)=1.
REWIND 3
REWIND 4
DO 7 LL=1,<
READ(3) (U(I),I=1,N1)
READ(4) (V(I),I=1,N)
Z1=0
DO 8 I=1,N
Z1=Z1+V(I)*X2(I)
8 CONTINUE
Z3=Z1/U(N1)
DO 9 I=1,N
9 X2(I)=X2(I)-Z3*V(I)
7 CONTINUE
DO 16 I=1,N
16 Y2(I)=0.
Y2(L)=1.
REWIND 3
REWIND 4
DO 17 LL=1,K
READ(3) (U(I),I=1,N1)
READ(4) (V(I),I=1,N)
Z1=0
DO 18 I=1,N
Z1=Z1+U(I)*Y2(I)
18 CONTINUE
Z3=Z1/U(N1)
DO 19 I=1,N
19 Y2(I)=Y2(I)-Z3*U(I)
27 CONTINUE
L3=L2+1
17 CONTINUE
15 CONTINUE
DO 40 I=1,N
X2(I)=X2(I)/S1
4 Y2(I)=Y2(I)/S2
S3=0
DO 20 I=1,N
20 S3=S3+X2(I)*Y2(I)
IF (S3.LT.EPS) GOTO 27
X2(N1)=S3
WRITE(3) (X2(I),I=1,N1)
WRITE(4) (Y2(I),I=1,N)
97 CONTINUE
RETURN
END
```



References

- [1] J.Gergely: Inversion of Large-Scale Sparse Matrices, Pubblicazioni Istituto per le applicazioni del Calcolo Serie III, N.158, Roma, 1978.
- [2] J.Gergely: Numerical methods for sparse matrices, treatise, Budapest, 1974. /in Hungarian/.
- [3] J.K.Reid: FORTRAN subroutines for handling sparse linear programming bases, Oxfordshire, 1976.
- [4] J.K.Reid: Sparse Matrices, York, 1976.
- [5] Peters and J.H.Wilkinson: Eigenvalues of  $Ax = \lambda Bx$  with band symmetric A and B, Com.J.12. 398-404.
- [6] J.S.Duff: A survey of Sparse Matrix Research, Proceedings of the IEEE, vol.65, No.4.1977.
- [7] A Dold and B.Eckmann: Sparse Matrix Techniques, Springer, Copenhagen, 1976.
- [8] B.M.Irons: A frontal solution program for finite element analysis, Int.J.Numer.Methods Eng., v.2. 5-32.
- [9] R.P.Tewarson: Sparse Matrices, Academic Press, New York and London, 1973.
- [10] J.H.Wilkinson: The Algebraic eigenvalue problem, Clarendon Press, Oxford, 1965.

99/1979 Ivics József: KGST Riga

100/1979 Téli iskola

1980-ban jelentek meg:

- 101/1980 Gerencsér László - Hangos Katalin:  
Diszkrét lineáris sztochasztikus rendszerek  
önhangoló szabályozása
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Az SDLA előzetes ismertetése
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Preliminary description of SDLA
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Relációs adatbázis logikai szintű vizsgálata  
funkcionális függőségek szempontjából
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Tanulmányok a statisztikai adatfeldolgozásról
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114/1980	Demetrovics János: Relációs adatmodell logikai és strukturális vizsgálata





